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High-dimensional neural-network potentials for multicomponent systems: Applications to zinc oxide

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Artificial neural networks represent an accurate and efficient tool to construct high-dimensional potential-energy surfaces based on first-principles data. However, so far the main drawback of this method has been the limitation to a single atomic species. We present a generalization to compounds of arbitrary chemical composition, which now enables simulations of a wide range of systems containing large numbers of atoms. The required incorporation of long-range interactions is achieved by combining the numerical accuracy of neural networks with an electrostatic term based on environment-dependent charges. Using zinc oxide as a benchmark system we show that the neural network potential-energy surface is in excellent agreement with density-functional theory reference calculations, while the evaluation is many orders of magnitude faster.

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